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Oxygen and Carbon Substrate Concentrations in Microbial Floc Particles by the Adomian Decomposition Method

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Abstract

In this paper, we solve a system of two coupled nonlinear differential equations that determine the concentrations of oxygen and the carbon substrate. This system models the excess sludge production from water treatment plants. We will apply the Adomian decomposition method combined with the Duan–Rach modified recursion scheme for analytical approximations of oxygen and the carbon substrate. Our graphs of the objective error analysis demonstrate the rapid rate of convergence of our sequence of analytic approximate solutions without recourse to comparisons with an alternate solution technique. The Adomian decomposition method yields a rapidly convergent, easily computable and readily verifiable sequence of analytic approximations that are convenient for parametric simulations.

1 Introduction

The disposal of excess sludge from waste water treatment plants represents a rising challenge in designing activated sludge processes [1–4]. Sludge comes as semi-solid material left from waste water treatment plants, or sometimes sludge comes as solids removed from the raw water. The sludge will become putrescent in a short time once anaerobic bacteria take over, and must be removed from the sedimentation tank before this can happen. Tyagi et al. [4] discussed the dynamic behavior of activated sludge. Abbassi et al. [2] developed a mathematical model that describes substrate removal, oxygen utilization and excess sludge production within a microbial floc particle, surrounded by a biodegradable substrate [3].

In [3], a mathematical model that relates the concentration of the carbon substrate and the concentration of oxygen was established as a system of two coupled Lane–Emden type equations

$$\frac{d^2u}{d\rho^2}+\frac{2}{\rho}\frac{du}{d\rho} = -\alpha_2+F_1\left(u(\rho),v(\rho)\right)\,, \tag{1}$$

$$\frac{d^2v}{d\rho^2}+\frac{2}{\rho}\frac{dv}{d\rho} = F_2\left(u(\rho),v(\rho)\right)\,, \tag{2}$$

subject to two mixed sets of Neumann and Dirichlet boundary conditions

$$u'(0)=0,\ u(1)=1,\ v'(0)=0,\ v(1)=1\,, \tag{3}$$

where the functions $u(\rho)$ and $v(\rho)$ are the concentration of the carbon substrate and the concentration of oxygen, respectively, ρ is the radius of a spherical floc particle, and the system nonlinearities are

$$F_1\left(u\left(\rho\right),v\left(\rho\right)\right) = \alpha_1 f_1\left(u\left(\rho\right),v\left(\rho\right)\right)+\alpha_3 f_2\left(u\left(\rho\right),v\left(\rho\right)\right)\,, \tag{4}$$

$$F_2\left(u\left(\rho\right),v\left(\rho\right)\right) = \alpha_4 f_1\left(u\left(\rho\right),v\left(\rho\right)\right)+\alpha_5 f_2\left(u\left(\rho\right),v\left(\rho\right)\right)\,, \tag{5}$$

where

$$f_1\left(u\left(\rho\right),v\left(\rho\right)\right) = \frac{u\left(\rho\right)v\left(\rho\right)}{\left(l_1+u\left(\rho\right)\right)\left(m_1+v\left(\rho\right)\right)}\,, \tag{6}$$

$$f_2\left(u\left(\rho\right),v\left(\rho\right)\right) = \frac{u\left(\rho\right)v\left(\rho\right)}{\left(l_2+u\left(\rho\right)\right)\left(m_2+v\left(\rho\right)\right)}\,, \tag{7}$$

which are products of the respective Michaelis–Menten nonlinearities, i.e.

$$f_j\left(u\left(\rho\right),v\left(\rho\right)\right)=M_j\left(u\left(\rho\right)\right)\times M_j\left(v\left(\rho\right)\right)=\frac{u\left(\rho\right)}{l_j+u\left(\rho\right)}\times\frac{v\left(\rho\right)}{m_j+v\left(\rho\right)}\,, \tag{8}$$

for $j=1,2$, where M_j is the respective Michaelis–Menten nonlinear operator. Note that in [3], the parameter α_5 in Eq. (5) was denoted as a product $\alpha\,\alpha_5$.

In this work, we shall apply the Adomian decomposition method [5–11] combined with the Duan–Rach modified recursion scheme [12–14] to systematically obtain a rapidly convergent analytic approximate solution that is convenient for numerical simulations. The rapid rate of convergence of our approximate solutions is validated by graphs of the error analysis that features the error remainder functions and the maximal error remainder parameters instead of comparison to an alternate solution technique alone.

We remark that the Adomian decomposition method has been efficiently used to solve a wide variety of nonlinear problems in engineering and science [7–9, 15–20], especially including several in theoretical chemistry [3, 11, 14, 21–24].

2 The Duan–Rach modified recursion scheme in the Adomian decomposition method

We rewrite Eqs. (1) and (2) in Adomian's operator-theoretic form as

$$Lu = -\alpha_2 + F_1(u(\rho), v(\rho)) \,, \tag{9}$$

$$Lv = F_2(u(\rho), v(\rho)) \,, \tag{10}$$

where the linear differential operator L is defined as

$$Lw(\rho) = \frac{d^2}{d\rho^2} w(\rho) + \frac{2}{\rho}\frac{d}{d\rho} w(\rho) \,. \tag{11}$$

Define the corresponding inverse operator L^{-1} [25, 26]

$$L^{-1}w(\rho) = \int_0^\rho \left(r - \frac{r^2}{\rho}\right) w(r)dr \,, \tag{12}$$

we have [25, 26]

$$L^{-1}Lu = u(\rho) - u(0) \,, \; L^{-1}Lv = v(\rho) - v(0) \,, \tag{13}$$

for $\frac{du}{d\rho}(0) = 0$, and $\frac{dv}{d\rho}(0) = 0$.

Applying the corresponding inverse linear operator $L^{-1}(\cdot)$ to both sides of Eqs. (9) and (10) leads to

$$u(\rho) = u(0) - \frac{\alpha_2}{6}\rho^2 + L^{-1}F_1(u(\rho), v(\rho)) \,, \tag{14}$$

$$v(\rho) = v(0) + L^{-1}F_2(u(\rho), v(\rho)) \,, \tag{15}$$

which is a system of coupled nonlinear Volterra integral equations with two – as yet undetermined – constants of integration $u(0)$ and $v(0)$ as an intermediate step.

Denote

$$L_1^{-1}w(\rho) := [L^{-1}w(\rho)]_{\rho=1} = \int_0^1 \left(r - r^2\right) w(r)dr \,. \tag{16}$$

Substituting the boundary conditions $u(1)=1$ and $v(1)=1$ into Eqs. (14) and (15) we have

$$\begin{aligned} u(0) &= 1+\frac{\alpha_2}{6}-L_1^{-1}F_1\left(u(\rho),v(\rho)\right)\,, && (17)\\ v(0) &= 1-L_1^{-1}F_2\left(u(\rho),v(\rho)\right)\,. && (18)\end{aligned}$$

Substituting Eqs. (17) and (18) into Eqs. (14) and (15), we obtain the equivalent system of coupled nonlinear Fredholm-Volterra integral equations without any undetermined constants of integration as

$$\begin{aligned} u(\rho) &= 1+\frac{\alpha_2}{6}-\frac{\alpha_2}{6}\rho^2-L_1^{-1}F_1\left(u(\rho),v(\rho)\right)+L^{-1}F_1\left(u(\rho),v(\rho)\right)\,, && (19)\\ v(\rho) &= 1-L_1^{-1}F_2\left(u(\rho),v(\rho)\right)+L^{-1}F_2\left(u(\rho),v(\rho)\right)\,. && (20)\end{aligned}$$

Next we apply the respective Adomian decomposition series

$$u(\rho)=\sum_{n=0}^{\infty}u_n(\rho),\quad v(\rho)=\sum_{n=0}^{\infty}v_n(\rho), \tag{21}$$

$$F_1\left(u(\rho),v(\rho)\right)=\sum_{n=0}^{\infty}A_{1,n}(\rho),\quad F_2\left(u(\rho),v(\rho)\right)=\sum_{n=0}^{\infty}A_{2,n}(\rho), \tag{22}$$

$$f_1\left(u(\rho),v(\rho)\right)=\sum_{n=0}^{\infty}B_{1,n}(\rho),\quad f_2\left(u(\rho),v(\rho)\right)=\sum_{n=0}^{\infty}B_{2,n}(\rho), \tag{23}$$

where the two-variable Adomian polynomials satisfy

$$A_{1,n}=\alpha_1B_{1,n}+\alpha_3B_{2,n},\quad A_{2,n}=\alpha_4B_{1,n}+\alpha_5B_{2,n}, \tag{24}$$

$$\begin{aligned} B_{1,0} &= \frac{u_0v_0}{(l_1+u_0)(m_1+v_0)}, && (25)\\ B_{1,1} &= \frac{m_1{u_0}^2v_1+l_1u_1{v_0}^2+m_1l_1\left(u_1v_0+u_0v_1\right)}{(l_1+u_0)^{2}(m_1+v_0)^{2}},\ \ldots, && (26)\end{aligned}$$

from Eqs. (4), (5), (6) and (7), and replacing $m_1\to m_2$ and $l_1\to l_2$ in $B_{1,n}$ leads to $B_{2,n}$.

The two-variable Adomian polynomials for the general bivariate function $f(u,v)$ are defined by the formula [5]

$$A_n=A_n(u_0,u_1,\cdots,u_n;v_0,v_1,\cdots,v_n)=\frac{1}{n!}\frac{d^n}{d\lambda^n}f\left(\sum_{j=0}^{n}u_j\lambda^j,\ \sum_{j=0}^{n}v_j\lambda^j\right)\Bigg|_{\lambda=0}\,. \tag{27}$$

Other algorithms for the one-variable and multivariable Adomian polynomials have been proposed such as in [5,9,10,27–35]. Duan [33–35] has recently crafted several new, more efficient algorithms for fast generation of the one-variable and multivariable Adomian polynomials. For convenience, we list the first five two-variable Adomian polynomials of the general bivariate function $f(u,v)$ with the decompositions $u=\sum_{n=0}^{\infty}u_n,\ v=\sum_{n=0}^{\infty}v_n$ as follows,

$$\begin{aligned}
A_0 &= f(u_0,v_0),\\
A_1 &= v_1 f^{(0,1)}(u_0,v_0)+u_1 f^{(1,0)}(u_0,v_0),\\
A_2 &= v_2 f^{(0,1)}+\tfrac{1}{2}v_1^2 f^{(0,2)}+u_2 f^{(1,0)}+u_1v_1 f^{(1,1)}+\tfrac{1}{2}u_1^2 f^{(2,0)},\\
A_3 &= v_3 f^{(0,1)}+v_1v_2 f^{(0,2)}+\tfrac{1}{6}v_1^3 f^{(0,3)}+u_3 f^{(1,0)}+\left(u_2v_1+u_1v_2\right) f^{(1,1)}+\tfrac{1}{2}u_1v_1^2 f^{(1,2)}\\
&\quad +u_1u_2 f^{(2,0)}+\tfrac{1}{2}u_1^2v_1 f^{(2,1)}+\tfrac{1}{6}u_1^3 f^{(3,0)},\\
A_4 &= v_4 f^{(0,1)}+\left(\tfrac{v_2^2}{2}+v_1v_3\right) f^{(0,2)}+\tfrac{1}{2}v_1^2v_2 f^{(0,3)}+\tfrac{1}{24}v_1^4 f^{(0,4)}+u_4 f^{(1,0)}\\
&\quad +\left(u_3v_1+u_2v_2+u_1v_3\right) f^{(1,1)}+\left(\tfrac{1}{2}u_2v_1^2+u_1v_1v_2\right) f^{(1,2)}+\tfrac{1}{6}u_1v_1^3 f^{(1,3)}\\
&\quad +\left(\tfrac{u_2^2}{2}+u_1u_3\right) f^{(2,0)}+\left(u_1u_2v_1+\tfrac{1}{2}u_1^2v_2\right) f^{(2,1)}+\tfrac{1}{4}u_1^2v_1^2 f^{(2,2)}+\tfrac{1}{2}u_1^2u_2 f^{(3,0)}\\
&\quad +\tfrac{1}{6}u_1^3v_1 f^{(3,1)}+\tfrac{1}{24}u_1^4 f^{(4,0)},
\end{aligned}$$

where we use the notation $f^{(m,n)}=f^{(m,n)}(u_0,v_0)=\frac{\partial^{m+n}f}{\partial u^m\partial v^n}(u_0,v_0)$ as a space-saving shorthand.

The MATHEMATICA code generating the two-variable Adomian polynomials of a general abstract function $f(u,v)$ based on the algorithm in Theorem 1 [35] is listed in the Appendix.

Upon substitution of the decompositions (21) and (22) into Eqs. (19) and (20), we obtain

$$\sum_{n=0}^{\infty}u_n(\rho)=1+\frac{\alpha_2}{6}-\frac{\alpha_2}{6}\rho^2-L_1^{-1}\sum_{n=0}^{\infty}A_{1,n}(\rho)+L^{-1}\sum_{n=0}^{\infty}A_{1,n}(\rho), \tag{28}$$

$$\sum_{n=0}^{\infty}v_n(\rho)=1-L_1^{-1}\sum_{n=0}^{\infty}A_{2,n}(\rho)+L^{-1}\sum_{n=0}^{\infty}A_{2,n}(\rho). \tag{29}$$

We establish the system of coupled Duan-Rach modified recursion schemes

$$\begin{gathered}
u_0(\rho)=1+\tfrac{\alpha_2}{6},\\
u_1(\rho)=-\tfrac{\alpha_2}{6}\rho^2-L_1^{-1}A_{1,0}(\rho)+L^{-1}A_{1,0}(\rho),\\
u_{n+2}(\rho)=-L_1^{-1}A_{1,n+1}(\rho)+L^{-1}A_{1,n+1}(\rho),\ n\geq 0,
\end{gathered} \tag{30}$$

$$\begin{gathered}
v_0(\rho)=1,\\
v_{n+1}(\rho)=-L_1^{-1}A_{2,n}(\rho)+L^{-1}A_{2,n}(\rho),\ n\geq 0.
\end{gathered} \tag{31}$$

Next we list the first calculated solution components as

$$\begin{aligned}
u_1(\rho) &= \frac{\alpha_2+6}{6}\left(\frac{\alpha_1}{(m_1+1)(\alpha_2+6l_1+6)}+\frac{\alpha_3}{(m_2+1)(\alpha_2+6l_2+6)}\right)(\rho^2-1)-\frac{\alpha_2\rho^2}{6},\\
v_1(\rho) &= \frac{\alpha_2+6}{6}\left(\frac{\alpha_4}{(m_1+1)(\alpha_2+6l_1+6)}+\frac{\alpha_5}{(m_2+1)(\alpha_2+6l_2+6)}\right)(\rho^2-1).
\end{aligned}$$

The approximate solution functions as defined by Adomian and co-workers are

$$\phi_{m+1}(\rho) = \sum_{n=0}^{m} u_n(\rho), \quad \psi_{m+1}(\rho) = \sum_{n=0}^{m} v_n(\rho), \ m \geq 0. \tag{32}$$

In order to evaluate the accuracy of our approximate solutions, we consider the error remainder functions

$$\begin{aligned} ER_{1,n}(\rho) &= \tfrac{d^2}{d\rho^2}\phi_n(\rho) + \tfrac{2}{\rho}\tfrac{d}{d\rho}\phi_n(\rho) + \alpha_2 - F_1(\phi_n(\rho), \psi_n(\rho)), \\ ER_{2,n}(\rho) &= \tfrac{d^2}{d\rho^2}\psi_n(\rho) + \tfrac{2}{\rho}\tfrac{d}{d\rho}\psi_n(\rho) - F_2(\phi_n(\rho), \psi_n(\rho)), \end{aligned} \tag{33}$$

and the maximal error remainder parameters

$$MER_{1,n} = \max_{0 \leq \rho \leq 1} |ER_{1,n}(\rho)|, \quad MER_{2,n} = \max_{0 \leq \rho \leq 1} |ER_{2,n}(\rho)|, \tag{34}$$

whenever the solutions are unknown in advance.

By the coupled system of the Duan-Rach modified recursion schemes in (30) and (31), we can easily calculate the solution components without any undetermined coefficients and including all of the modelling parameters. The results are shown to be superior for parametric simulations.

3 Numerical simulations

First, we assign $m_1 = l_1 = m_2 = l_2 = 0.0001$ as in [3]. We further specify α_1=5, α_2=1, α_3 =0.1, α_4=0.1, α_5=0.05 to examine the error remainder functions and the maximal error remainder parameters.

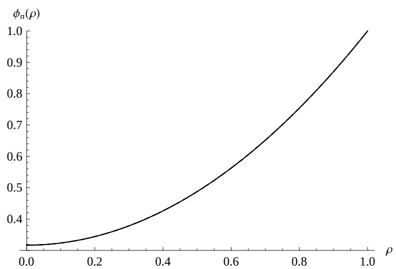

Fig. 1: Curves of the approximate solutions $\phi_n(\rho)$ versus ρ for $n = 2$ (solid line), $n = 3$ (dot line) and $n = 4$ (dash line).

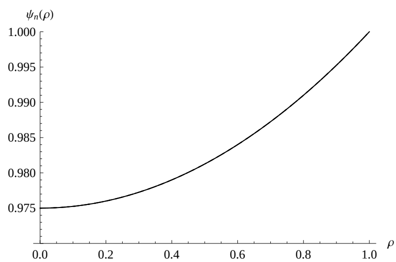

Fig. 2: Curves of the approximate solutions $\psi_n(\rho)$ versus ρ for $n = 2$ (solid line), $n = 3$ (dot line) and $n = 4$ (dash line).

In Figs. 1 and 2, we plot the curves of the approximate solutions $\phi_n(x)$ and $\psi_n(\rho)$ versus ρ for $n = 2, 3, 4$, respectively, where the three curves nearly overlap.

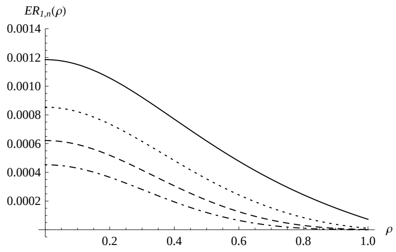

Fig. 3: Curves of the error remainder functions $ER_{1,n}(\rho)$ versus ρ for $n = 2$ (solid line), $n = 3$ (dot line), $n = 4$ (dash line) and $n = 5$ (dot-dash line).

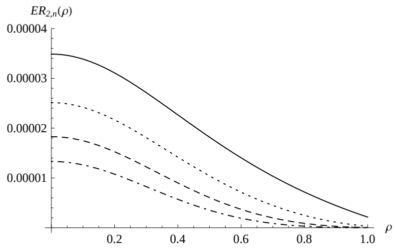

Fig. 4: Curves of the error remainder functions $ER_{2,n}(\rho)$ versus ρ for $n = 2$ (solid line), $n = 3$ (dot line), $n = 4$ (dash line) and $n = 5$ (dot-dash line).

Table 1: The Maximal error remainder parameters $MER_{1,n}$ and $MER_{2,n}$.

n	2	3	4	5	6	7
$MER_{1,n}$	0.00118506	0.000853760	0.000621465	0.000452526	0.000329508	0.000239928
$MER_{2,n}$	0.0000348547	0.0000251106	0.0000182784	0.0000133096	9.69142×10^{-6}	7.05670×10^{-6}

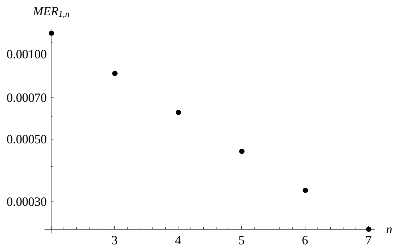

Fig. 5: Logarithmic plots of $MER_{1,n}$ versus n for $n = 2$ through 7.

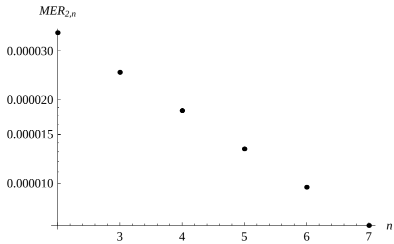

Fig. 6: Logarithmic plots of $MER_{2,n}$ versus n for $n = 2$ through 7.

The curves of the error remainder functions $ER_{1,n}(\rho)$ and $ER_{2,n}(\rho)$ versus ρ for $n = 2, 3, 4, 5$ are plotted in Figs. 3 and 4, respectively.

The maximal error remainder parameters $MER_{1,n}$ and $MER_{2,n}$, for $n = 2$ through 7, are listed in Table 1. The logarithmic plots of these values are displayed in Figs. 5 and 6, respectively, where the points almost lay on a straight line thus indicating an approximately exponential rate of convergence.

Then we use 6-term approximations to examine the effects of the parameters α_1, α_2, α_3, α_4, α_5 to the solution. In Figs. 7–9, the effects of $\alpha_2, \alpha_1, \alpha_3$ on the approximate solution $\phi_6(\rho)$ are shown, respectively. The approximate solution $\phi_6(\rho)$ increases with the increasing of α_2, but decreases with the increasing of α_1 or α_3.

We checked that the effects of $\alpha_1, \alpha_2, \alpha_3$ on the approximate solution $\psi_6(\rho)$ are very

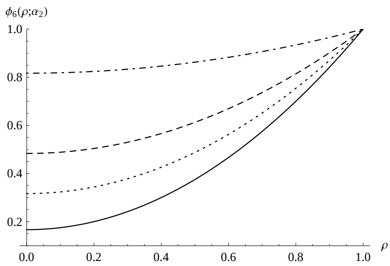

Fig. 7: Curves of the approximate solutions $\phi_6(\rho;\alpha_2)$ versus ρ for $\alpha_1 = 5$, $\alpha_3 = 0.1$, $\alpha_4 = 0.1$, $\alpha_5 = 0.05$ and for different values of α_2: 0.1 (solid line), 1 (dot line), 2 (dash line) and 4 (dot-dash line).

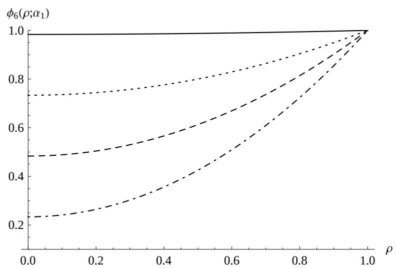

Fig. 8: Curves of the approximate solutions $\phi_6(\rho;\alpha_1)$ versus ρ for $\alpha_2 = 1$, $\alpha_3 = 0.1$, $\alpha_4 = 0.1$, $\alpha_5 = 0.05$ and for different values of α_1: 1 (solid line), 2.5 (dot line), 4 (dash line) and 5.5 (dot-dash line).

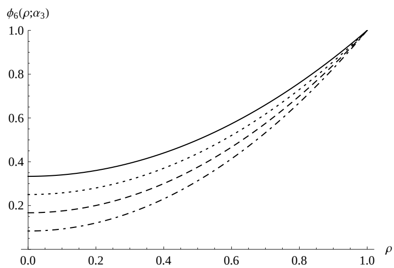

Fig. 9: Curves of the approximate solutions $\phi_6(\rho;\alpha_3)$ versus ρ for $\alpha_1 = 5$, $\alpha_2 = 1$, $\alpha_4 = 0.1$, $\alpha_5 = 0.05$ and for different values of α_3: 0.001 (solid line), 0.5 (dot line), 1 (dash line) and 1.5 (dot-dash line).

weak, and with the increasing of α_4 or α_5, the approximate solution $\psi_6(\rho)$ decreases, while $\phi_6(\rho)$ is nearly invariant.

Next, we assign α_1=5, α_2=1, α_3 =0.1, α_4=0.1, α_5=0.05 to examine the effects of the parameters l_i, m_i, $i = 1, 2$, on the solution.

In Figs. 10 and 11, we plot the curves of the approximate solutions $\phi_6(\rho)$ and $\psi_6(\rho)$ versus ρ for $m_1 = m_2 = l_2 = 0.0001$ and for different values of l_1. In Figs. 12 and 13, we plot the curves of the approximate solutions $\phi_6(\rho)$ and $\psi_6(\rho)$ versus ρ for $l_1 = m_2 = l_2 = 0.0001$ and for different values of m_1. The increasing of l_1 or m_1 leads to increasing the solutions. We checked that similar results hold for parameters l_2 and m_2.

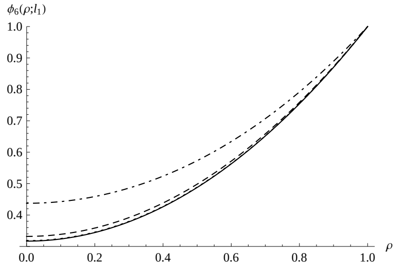

Fig. 10: Curves of the approximate solutions $\phi_6(\rho;l_1)$ versus ρ for $m_1 = m_2 = l_2 = 0.0001$ and for different values of l_1: 0.0001 (solid line), 0.001 (dot line), 0.01 (dash line) and 0.1 (dot-dash line).

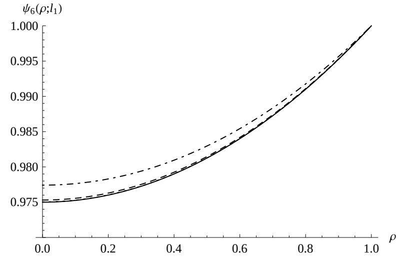

Fig. 11: Curves of the approximate solutions $\psi_6(\rho;l_1)$ versus ρ for $m_1 = m_2 = l_2 = 0.0001$ and for different values of l_1: 0.0001 (solid line), 0.001 (dot line), 0.01 (dash line) and 0.1 (dot-dash line).

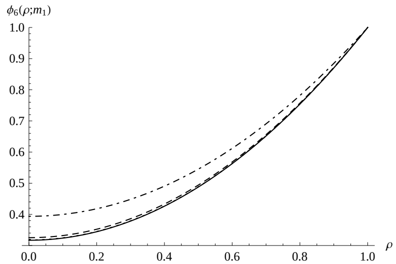

Fig. 12: Curves of the approximate solutions $\phi_6(\rho;m_1)$ versus ρ for $l_1 = m_2 = l_2 = 0.0001$ and for different values of m_1: 0.0001 (solid line), 0.001 (dot line), 0.01 (dash line) and 0.1 (dot-dash line).

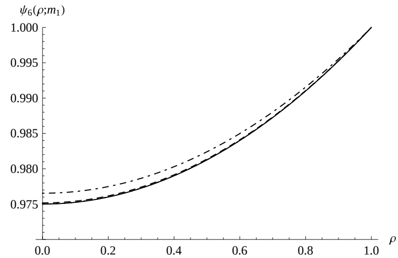

Fig. 13: Curves of the approximate solutions $\psi_6(\rho;m_1)$ versus ρ for $l_1 = m_2 = l_2 = 0.0001$ and for different values of m_1: 0.0001 (solid line), 0.001 (dot line), 0.01 (dash line) and 0.1 (dot-dash line).

4 Conclusions

In this work, we have examined microbial floc particles immersed in a system of the carbon substrate and oxygen. The system models the excess sludge production from water treatment plants. The proposed approach depends mainly on combining the Adomian method with the Duan-Rach modified recursion scheme. The work resulted in an approximation of the concentrations of carbon and the concentration of oxygen with a high level of accuracy. The evaluated approximations show enhancements over existing techniques where the minimal size of the obtained errors and the illustrated graphs emphasize these improvements.

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Appendix. MATHEMATICA code for the two-variable Adomian polynomials based on Theorem 1 [35].

```
Adth1[M_]:=Module[{},A[0]=f[Subscript[u, 0],Subscript[v, 0]];
For[n=1,n<=M,n++,A[n]=1/n*
Sum[(k+1)*(Subscript[u, k+1]*D[A[n-1-k],Subscript[u, 0]]
+Subscript[v, k+1]*D[A[n-1-k],Subscript[v, 0]]),{k,0,n-1}]];
Table[A[n],{n,0,M}]]
```

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